Comment on: "Using Ni Substitution and ^{17}O NMR to Probe the Susceptibility $\chi'(\mathbf{q})$ in Cuprates"

In a recent letter, Bobroff *et al.* [1] presented novel ^{17}O NMR measurements for $YBa_2(Cu_{1-x}Ni_x)_3O_{6+y}$. They observed a strong T-dependent broadening of the ^{17}O NMR-lines which they attributed to the oscillatory electron spin polarization induced by Ni impurities. Their experiment offers a new probe of the momentum dependence of the static spin susceptibility $\chi'(\mathbf{q})$, complementary to the NMR observation of the Gaussian component of the transverse relaxation time, $T_{2\mathrm{G}}$, of planar Cu [2].

To understand the strong T dependence of the NMR line width $\Delta\nu(T)$, Bobroff *et al.* performed calculations to simulate the NMR line shape by assuming a Gaussian form for the electron spin susceptibility $\chi'_{\mathrm{G}}(\mathbf{q}) = 4\pi\chi^*\xi^2 \exp[-(\mathbf{q}-\mathbf{Q})^2\xi^2]$ with $\mathbf{Q} = (\pi,\pi)$. They found that the ^{17}O line width $\Delta\nu$ is independent of the antiferromagnetic correlation length ξ. For the overdoped sample ($y = 1$), where $\Delta\nu = \chi^* f(\xi)$ is only very weakly T-dependent, they conclude that χ^* is basically T-independent. However, for the underdoped samples ($y = 0.6$) they find that the strong T-dependence of $\Delta\nu$ can *only* be explained with a T-dependent χ^*. Combining these results with the T-dependence of $T_{2G}^{-1} \sim \chi^*\xi$, they pointed out that this implies a T-independent ξ for the underdoped samples. They also remark that a Lorentzian model $\chi'_{\mathrm{L}}(\mathbf{q}) = 4\pi\chi^*\xi^2/(1+(\mathbf{q}-\mathbf{Q})^2\xi^2)$ gives similar results. This is in contradiction to the spin fluctuation scenario of cuprate superconductors [3], which is based on the Lorentzian form $\chi'_{\mathrm{L}}(\mathbf{q})$.

Stimulated by their experiment we also performed calculations to simulate the ^{17}O NMR lineshape. For the Gaussian susceptibility $\chi'_{\mathrm{G}}(\mathbf{q})$, we obtain the same results as Bobroff *et al.* However, we obtain a strong ξ dependence of the ^{17}O line width with the Lorentzian form of $\chi'_{\mathrm{L}}(\mathbf{q})$. Our results using $\chi'_{\mathrm{L}}(\mathbf{q})$ are shown in Fig. 1, where we plot the ξ-dependence of $\Delta\nu$. Due to the $1/T$ dependence of the Ni magnetic moment, $\Delta\nu$ corresponds to $T\Delta\nu_{\mathrm{imp}}$ in Ref. [1]. The inset shows our results for $\chi'_{\mathrm{G}}(\mathbf{q})$. Our results obtained with $\chi'_{\mathrm{L}}(\mathbf{q})$ (curve *(a)*) demonstrate that the experimental results of Bobroff *et al.* are clearly compatible with a T-dependent ξ [3]. Furthermore, including in addition to the nearest neighbor Cu-O hyperfine coupling C a next-nearest neighbor coupling C' [4] (curves *(b), (c)* and *(d)*) we obtain a flattening of $\Delta\nu(\xi)$ for $\xi = 1..2$. This provides a possible explanation for the different behavior of overdoped ($\xi = 1..2$) and underdoped ($\xi = 2..4$) systems.

Due of the location of the ^{17}O between two ^{63}Cu sites, the local field at the ^{17}O site behaves as $\sim \partial\tilde{\chi}(r)/\partial r$, where $\tilde{\chi}(r)$ is the envelope of the real space susceptibility (see Fig. 4 in Ref. [1]). Our analytical computations show that for the Gaussian form $\chi'_{\mathrm{G}}(\mathbf{q})$, $\Delta\nu(\xi)$ is approximately constant for a realistic range of ξ. For the Lorentzian form $\chi'_{\mathrm{L}}(\mathbf{q})$, $\Delta\nu(\xi) \sim \xi^{3/2}$, in agreement with our numerical results (see solid line in Fig. 1).

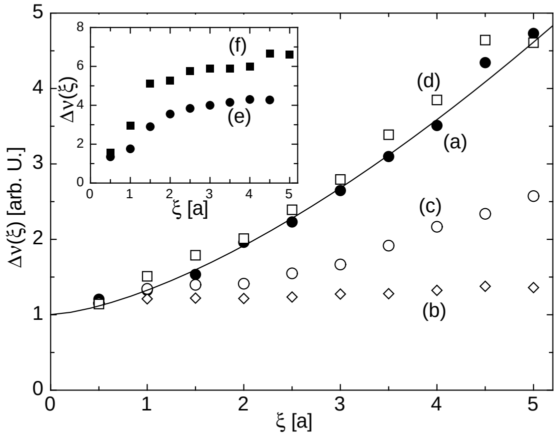

FIG. 1. The ^{17}O linewidth $\Delta\nu$ as a function of ξ. Curve *(a)* shows the result for $x = 2\%$ Ni doping and $C' = 0$. The solid line is a fit with $\Delta\nu = 1.0 + 0.32\xi^{3/2}$. Curves *(b), (c)* and *(d)* correspond to $x = 0.5, 2$ and 4% Ni doping, respectively and $C'/C = 0.25$. The inset represents the results for $\chi'_{\mathrm{G}}(\mathbf{q})$ with *(e)* $x = 2\%$ and *(f)* $x = 4\%$ Ni doping.

Taking the T_{2G} data from [5] (corrected for T_1 contributions [6]) and $T\Delta\nu$ for the underdoped sample from [1], we computed the product $T_{2G}T\Delta\nu$, which is independent of χ^*, and *which for any form of* $\chi'(q)$ depends solely on ξ. In contrast to [1] we find that this product is strongly T-dependent, dropping by more than a factor of 2 between $100\,K$ and $200\,K$. For a Gaussian this implies that ξ increases as T increases, an unreasonable result. For a Lorentzian, ξ decreases with increasing T. We therefore believe that a Gaussian form of $\chi'(q)$ is unlikely.

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